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TECHNICAL NOTE 2439

A THEORY OF CONDUCTIVITY OF COLD-WORKED COPPER

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A THEORY OF CONDUCTIVITY OF COLD-WORKED COPPER

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SUMMARY

The increase in the resistivity of copper under cold-working is calculated. The increase is assumed to be caused by dislocations surrounded by a long-range electrostatic field that scatters the conduction electrons. The amount of scattering is found by the method of deformation potentials of Bardeen and Shockley. The scattering is present in addition to the normal thermal scattering and is regarded as a perturbation in the Boltzmann equation. This perturbation is used to find the incremental resistance per dislocation. From this calculated increment in resistance and the known increase of resistivity of heavily cold-worked copper, the number of dislocations in the cold-worked copper is found to be in agreement with the number estimated on the basis of stored-energy measurements.

INTRODUCTION

In the vicinity of an edge-type dislocation, a metal is strained. A dilation of the lattice is associated with this strain; therefore the density of electrons varies in the vicinity of the dislocation and the width of the filled portion of the conduction band must also vary. In equilibrium, however, the top of the filled portion of the conduction band must be at the same level everywhere; so the bottom of the conduction band must accommodate the variation. This variation scat[illegible] electrons and is taken into account in the ensuing calculation.

The matrix elements for this scattering are calculated by the method of deformation potentials of Bardeen and Shockley (reference 1). Once these matrix elements have been obtained, the rest of the calculation follows the method of Mackenzie and Sondheimer (reference 2), which treats the scattering due to dislocations as a small perturbation in the Boltzmann equation. This treatment gives the change of resistance at high temperatures, where the increment is only a few percent of the normal thermal resistance. An earlier calculation by Koehler (reference 3) deals with the resistance of cold-worked copper at absolute zero.

The physical motivation for this calculation and the results have been published in reference 4, whereas the detailed procedure is given in this report.

ANALYSIS

In order to discuss electronic motion in the vicinity of an edge dislocation, a coordinate system must be defined. The z-axis is taken to be the dislocation axis and the distance of a point from this axis is denoted by r_t. The angle of elevation above the slip plane is 2224
measured by θ. The dislocation will be taken to be positive, so that there will be an extra plane of atoms above the slip plane at $\theta = \pi/2$. The slip direction $\theta = 0$ is considered parallel to the x-axis. (Symbols are listed in appendix A.)

The density of ions varies near the dislocation. If n_0 is the density of ions in the unstrained metal and if Δn is the increment in the number of ions per unit volume then, as shown in appendix B,

$$\frac{\Delta n}{n_0} = \frac{a}{2\pi} \frac{(1-\nu-2\nu^2)}{(1-\nu^2)} \frac{\sin \theta}{r_t} \tag{1}$$

where a is the slip distance, and ν is Poisson's ratio. The width of the filled portion of the conduction band occupied by n electrons with effective mass m^* is

$$E_B = \frac{h^2}{2m^*}\left(\frac{3n}{8\pi}\right)^{2/3} \tag{2}$$

Not only n, but also m^* is a function of position in the neighborhood of the dislocation.

When two different metals are brought into contact, an electrostatic field is set up so that their Fermi levels are brought together. The bottom levels of the two conduction bands are then at different energies, the difference being equal to the difference in the width of the conduction bands. In a dislocation, regions of the metal subject to different strains are in contact with each other; in the same way as in the case of different metals it can then be expected that the Fermi levels are brought together in the vicinity of the dislocation, and that the variation in band width gives rise to a variation in the energy of the lower band edge.

The method of deformation potentials (reference 1) describes the most general method by which electronic motion in deformed crystals may be treated. Let ψ_0 be the wave function at the lower band edge. Let $\delta U(\vec{r})$ be the deviation of the lower band edge from its normal position. Then the wave function for an electron with energy E is given by $A(\vec{r})\ \psi_0(\vec{r})$ where A satisfies

$$\left[\frac{h^2}{2m^*(\vec{r})} \nabla^2 + \delta U(\vec{r})\right] A(\vec{r}) = EA(\vec{r}) \tag{3}$$

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or

$$\left[\frac{h^2}{2m_0{}^*} \nabla^2 + \frac{m^*}{m_0{}^*} (E-\delta U)\right] A(\vec{r}) = 0 \tag{4}$$

where $m_0{}^*$ is the effective mass in the undistorted lattice. Since $\psi_0(\vec{r})$ is taken to be the same for all wave functions in the band, it need not be considered and only the perturbation in $A(\vec{r})$ due to the dislocation must be evaluated.

Now, for an electron near the top of the filled portion of the conduction band, $E-\delta U$ is the width of the conduction band given by equation (2); hence

$$\frac{m^*}{m_0{}^*} (E-\delta U) = \frac{h^2}{2m_0{}^*}\left(\frac{3n}{8\pi}\right)^{2/3} \tag{5}$$

Setting $n = n_0 + \Delta n$ gives, to the first order in Δn

$$\frac{m^*}{m_0{}^*} (E-\delta U) = \frac{h^2}{2m_0{}^*}\left(\frac{3n_0}{8\pi}\right)^{2/3} + \frac{2}{3}\ \frac{h^2}{2m_0{}^*}\left(\frac{3n_0}{8\pi}\right)^{2/3}\left(\frac{\Delta n}{n_0}\right) \tag{6}$$

The second term on the right-hand side represents a perturbation due to the elastic distortion of the metal. Using equation (1) gives the perturbation as

$$\frac{2}{3}\left[\frac{h^2}{2m_0{}^*}\left(\frac{3n}{8\pi}\right)^{2/3}\right] \frac{a}{2\pi}\ \frac{(1-\nu-2\nu^2)}{(1-\nu^2)}\ \frac{\sin\theta}{r_t} \tag{7}$$

or

$$\frac{2}{3}\ E_{B,0}\ \frac{a}{2\pi}\ \frac{(1-\nu-2\nu^2)}{(1-\nu^2)}\ \frac{\sin\theta}{r_t} \tag{8}$$

where $E_{B,O}$ is the width of the filled portion of the conduction band in the unstrained metal. Therefore $A(\vec{r})$ is to be determined from the equation

$$\left[\frac{\hbar^2}{2m_O^*}\nabla^2 + E_{B,O} + E_{B,O}\frac{a}{3\pi}\frac{(1-\upsilon-2\upsilon^2)}{(1-\upsilon^2)}\frac{\sin\theta}{r_t}\right]A(\vec{r}) = 0 \tag{9}$$

The unperturbed equation is

$$\left[\frac{\hbar^2}{2m_O^*}\nabla^2 + E_{B,O}\right]A_O(\vec{r})$$

and its solution is $A_O(\vec{r}) = e^{i\vec{k}\cdot\vec{r}}$, where

$$\frac{\hbar^2|\vec{k}|^2}{2m_O^*} = E_{B,O}$$

and $A_O(\vec{r})$ is the factor that modulates $\psi_O(\vec{r})$, for an electron at the top of the conduction band, in the undeformed metal. The probability of transitions to states of the type

$$A(\vec{r}) = e^{i\vec{k}'\cdot\vec{r}}$$

must now be calculated. The new state has the same energy as the initial state

$$\frac{\hbar^2|\vec{k}'|^2}{2m_O} = E_{B,O}$$

but represents the scattered electron traveling in a new direction. From this scattering probability, the increase in resistance can be found by the method of reference 2.

Note that it is not necessary to know $m^*(r)$, but that it is only the variation of $n(r)$ that matters; $m^*(r)$ need not be known.

Equation (9) is the wave equation that a free particle of mass m_O^*, incident energy $E_{B,O}$, and charge $-q$ obeys, if scattered by an electrostatic potential

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$$V_e = \frac{a}{3\pi q}\frac{(1-\nu-2\nu^2)}{(1-\nu^2)}\frac{\sin\theta}{r_t}.$$

This is the potential of a line dipole located along the dislocation axis.

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CALCULATION OF MATRIX ELEMENTS

The perturbing potential in equation (9) has the form

$$V' = \beta\frac{\sin\theta}{r_t} \qquad (10)$$

where

$$\beta = \frac{2}{3}\frac{a}{2\pi}\frac{(1-\nu-2\nu^2)}{(1-\nu^2)}E_{B,0} \qquad (11)$$

This potential is assumed to exist in a rectangular box of length L along the dislocation axis and of area d^2 measured in a cross section perpendicular to the length L of the box. The unperturbed wave functions are normalized for this box, are selected to satisfy periodic boundary conditions, and are of the form

$$A_0(\vec{r}) = \frac{1}{\sqrt{V}}e^{i\vec{k}\cdot\vec{r}} \qquad (12)$$

where $V = Ld^2$ and is the volume of the box.

The matrix element of interest is

$$\frac{1}{V}\int_V e^{i(\vec{k}'-\vec{k})\cdot r}\,\beta\,\frac{\sin\theta}{r_t}\,dV \qquad (13)$$

which vanishes unless $k_z = k_z'$. Let $\vec{k}_t$, $\vec{k}_t'$, and $\vec{r}_t$ represent the components of $\vec{k}$, $\vec{k}'$, and $\vec{r}$, respectively, that are perpendicular to the dislocation axis. After integration along the z-axis, expression (13) becomes (if $k_z = k'_z$)

$$\frac{1}{d^2}\int_\lambda e^{i(\vec{k}_t'-\vec{k}_t)\cdot\vec{r}}\beta\,\frac{\sin\theta}{r_t}\,d\lambda \tag{14}$$

where $d\lambda$ is an element of surface of a plane perpendicular to the dislocation axis. Let the magnitude of $(\vec{k}_t-\vec{k}_t')$ be denoted by κ and the angle it makes with the slip plane by θ_0. Then the matrix element in question becomes

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$$\frac{1}{d^2}\int_\lambda e^{i\kappa r_t\cos(\theta-\theta_0)}\beta\,\frac{\sin\theta}{r_t}\,d\lambda \tag{15}$$

Setting $\theta-\theta_0=\alpha$ gives

$$\frac{1}{d^2}\int_\lambda e^{i\kappa r_t\cos\alpha}\,\frac{\beta}{r_t}\sin(\alpha+\theta_0)\,d\lambda \tag{16}$$

where $\sin(\alpha+\theta_0)$ can be expanded as

$$\sin\alpha\cos\theta_0+\cos\alpha\sin\theta_0 \tag{17}$$

The first term of expression (17) is odd in α. Because the exponential is even in α, this contribution to the integral vanishes. The remaining integrand gives

$$\beta\,\frac{\sin\theta_0}{d^2}\int_\lambda e^{i\kappa r_t\cos\alpha}\cos\alpha\,d\alpha\,dr_t \tag{18}$$

The integration over r_t from $r_t=0$ to $r_t=\infty$ can be performed by assuming that κ has a small positive imaginary part and then letting this imaginary part approach zero. This procedure gives for the matrix element

$$M(\vec{k},\vec{k}')=\frac{\beta\sin\theta_0}{d^2}\int\frac{1}{i\kappa}\,d\alpha \tag{19}$$

$$=\frac{2\pi\beta\sin\theta_0}{i\kappa\,d^2} \tag{20}$$

Let θ_t' and θ_t be the angles that $\vec{k}_t'$ and $\vec{k}_t$ (final and initial wave vectors, respectively) make with the slip plane. Then

$$\left|M(\vec{k},\vec{k}')\right|^2 = \frac{4\pi^2\beta^2}{d^4 k_t^2} \frac{\cos^2\left(\frac{\theta_t'+\theta_t}{2}\right)}{\sin^2\left(\frac{\theta_t'-\theta_t}{2}\right)} \tag{21}$$

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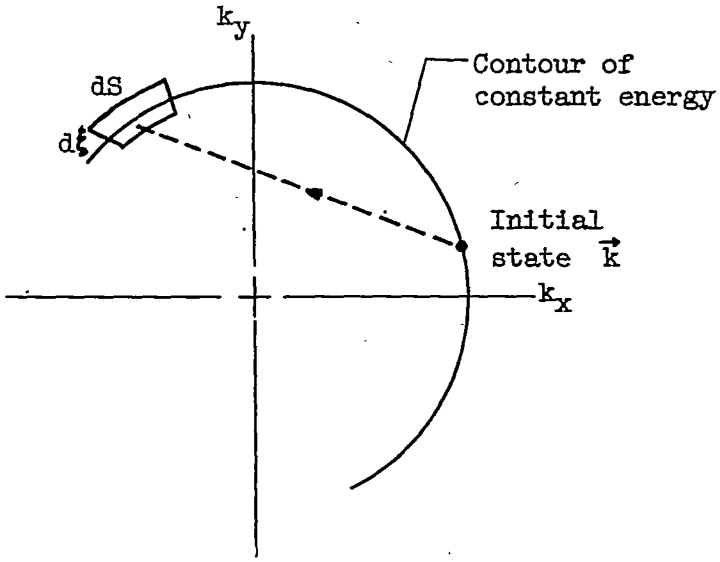
if $\left|\vec{k}_t'\right| = \left|\vec{k}_t\right|$.



Now consider this transition in $\vec{k}_t$ space, as shown in this figure. The plane represents all the states with a given value of k_z. The curve represents a contour of constant energy. As is usual in calculations of this type, the only transitions that are important are those that almost conserve energy. The electron is assumed in an initial state specified by $\vec{k}_t$. The quantity needed is the transition probability to the set of states in the element $dS\, d\xi$. The reasoning used here follows that given in reference 5.

If E_k' is the energy of the final state and E_k is the energy of the initial state, the probability that the electron will be in state $\vec{k}'$ after time t is

$$|a_{k}'|^2 = \frac{1}{\hbar^2} M(\vec{k},\vec{k}')^2 \frac{2(1-\cos pt)}{p^2} \tag{22}$$

where $p = (E_{k}'-E_{k})/\hbar$. Now the number of states per unit area of this two-dimensional $\vec{k}_t$ space is $\frac{d^2}{4\pi^2}$, and the probability of finding the electron in $dS\, d\xi$ is therefore $\frac{d^2}{4\pi^2} |a_{k}'|^2\, dS\, d\xi$. The total probability for finding the electron in dS is

$$dS \frac{d^2}{4\pi^2} \int |a_{k}'|^2 \, d\xi \tag{23}$$

The matrix element $M(\vec{k},\vec{k}')$ can be assumed constant over the range of $d\xi$. The only important contributions to the integrand come from small values of ξ for which

$$p = \frac{1}{\hbar} \frac{\partial E}{\partial \xi} \xi \tag{24}$$

where ξ is taken to be zero on the contour of constant energy shown in the preceding figure. The quantity actually needed is the probability of transition per unit time. This differentiation then gives

$$P(\vec{k},\vec{k}')\, dS = \frac{2\pi}{\hbar} \frac{\beta^2}{k_t^2 d^2} \frac{\cos^2\left(\frac{\theta_t'+\theta_t}{2}\right)}{\cos^2\left(\frac{\theta_t'-\theta_t}{2}\right)} \frac{dS}{\frac{dE}{d\xi}} \tag{25}$$

Now this probability of transition is superposed on the transition probability arising from the thermal vibrations of the lattice. In the normal metal, in the annealed state, and in the presence of an electric field, there is a deviation $g(\vec{k})$ from the Fermi distribution. This deviation is limited by the thermal scattering, the amount of the deviation determining the amount of the current. Cold working changes the conductivity of nonporous and isotropically conducting metals by only a few percent. In the presence of the field, the dislocation, and the thermal scattering, the deviation from the Fermi distribution is of the form $g(\vec{k}) - g_1(\vec{k})$, where g_1 is a small perturbation and $g(\vec{k})$ is the deviation that exists without the dislocation. Let $f_0(\vec{k})$ stand for the probability that the state associated with wave vector $\vec{k}$ is occupied according to the Fermi distribution:

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$$f_0(\vec{k}) = \frac{1}{1 + e^{\left[E(\vec{k}) - \zeta\right]/kT}} \tag{26}$$

Let $f(\vec{k})$ stand for the actual distribution, $f(\vec{k}) = f_0(\vec{k}) + g(\vec{k}) - g_1(\vec{k})$. The rate at which $f(\vec{k})$ changes because of an electric field in the x direction is

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$$\frac{\partial f}{\partial t} = \frac{df_0}{dk} \frac{k_x}{k} \frac{qF}{\hbar} \tag{27}$$

where F is the field, and where the surfaces of constant energy are assumed to be spheres in $\vec{k}$ space. Furthermore, the conduction process in the annealed metal will be assumed describable by a relaxation time time τ (references 2 and 5) so that

$$g(\vec{k}) = \frac{df_0}{dk} \frac{k_x}{k} \frac{qF}{\hbar} \tau = \frac{\partial f_0}{\partial k_t} \frac{k_x}{k_t} \frac{qF}{\hbar} \tau \tag{28}$$

In equilibrium, $\partial f/\partial t = 0$. The rate of change of f due to the field as given by equation (27), must therefore be balanced by the scattering. The rate of scattering due to the thermal vibrations is given by

$$\frac{\partial f}{\partial t} = - \frac{(f-f_0)}{\tau} = - \frac{g}{\tau} + \frac{g_1}{\tau} \tag{29}$$

and the rate of scattering due to the dislocation is

$$\frac{\partial f(\vec{k})}{\partial t} = \int \left[f(\vec{k}') - f(\vec{k})\right] P(\vec{k},\vec{k}')\, dS' \tag{30}$$

or

$$\begin{aligned}\frac{\partial f(k)}{\partial t} = &\int \left[f_0(\vec{k}') - f_0(\vec{k})\right] P(\vec{k},\vec{k}')\, dS' \\ &+ \int \left[g(\vec{k}') - g(\vec{k})\right] P(\vec{k},\vec{k}')\, dS' \\ &- \int \left[g_1(\vec{k}') - g_1(\vec{k})\right] P(\vec{k},\vec{k}')\, dS'\end{aligned} \tag{31}$$

In each integral occurring in equation (31) the integration is over the circle defined by $|k_t'| = |k_t|$, which lies in the plane $k_z' = k_z$.

The first integral vanishes because $f_0(\vec{k}) = f_0(\vec{k'})$; the last integral is neglected. Both $g_1(\vec{k})$ and $P(\vec{k},\vec{k'})$ are proportional to the perturbation represented by the dislocation. The last integral is therefore of second order in the perturbation. The total rate of change is

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$$\frac{df_0}{dk}\frac{k_x}{k}\frac{qF}{\hbar} - \frac{g}{\tau} + \frac{g_1}{\tau} + \int\left[g(\vec{k'}) - g(k)\right]P(\vec{k},\vec{k'})\,dS' = 0 \tag{32}$$

According to equation (28) the first two terms cancel. The remaining equation gives

$$g_1 = -\tau\int\left[g(\vec{k'}) - g(\vec{k})\right]P(\vec{k},\vec{k'})\,dS' \tag{33}$$

where g is given by equation (28).

Substituting from equation (28), the solution for g_1 becomes

$$g_1(\vec{k}) = \tau^2\frac{\partial f_0}{\partial k_t}\frac{qF}{\hbar}\int(\cos\,\theta_t - \cos\,\theta_t')\,P(\vec{k'},\vec{k})\,dS' \tag{34}$$

The value of $P(\vec{k'},\vec{k})\,dS'$ is given by equation (25). Substituting this value in equation (34) gives

$$g_1(\vec{k}) = \tau^2\frac{\partial f_0}{\partial k_t}\frac{qF}{\hbar}\frac{2\pi}{\hbar}\frac{\beta^2}{k_t^2}\frac{1}{d^2}\frac{1}{\frac{\partial E}{\partial k_t}}\int(\cos\,\theta_t - \cos\,\theta_t')\frac{\cos^2\left(\frac{\theta_t+\theta_t'}{2}\right)}{\sin^2\left(\frac{\theta_t-\theta_t'}{2}\right)}\,dS' \tag{35}$$

Now $dS' = k_t\,d\theta_t'$. Therefore

$$g_1(\vec{k}) = \tau^2\frac{\partial f_0}{\partial k_t}\frac{1}{k_t}\frac{qF}{\hbar^2}\frac{2\pi\beta^2}{d^2}\frac{1}{\frac{\partial E}{\partial k_t}}\int(\cos\,\theta_t - \cos\,\theta_t')\frac{\cos^2\left(\frac{\theta_t'+\theta_t}{2}\right)}{\sin^2\left(\frac{\theta_t'-\theta_t}{2}\right)}\,d\theta_f \tag{36}$$

From this change in electron distribution, the change in the current density can be determined:

$$\Delta j = \iiint q v_x \frac{2 g_1(k)}{2\pi^3} \, d\tau_{\vec{k}} \tag{37}$$

The electron velocity is given by

$$v_x = \frac{1}{\hbar} \frac{\partial E}{\partial k_t} \cos \theta_t \tag{38}$$

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and furthermore

$$d\tau_{\vec{k}} = k^2 \sin \gamma \, d\gamma \, d\theta_t \, dk \tag{39}$$

where γ is the angle that the $\vec{k}$ vector makes with the dislocation axis. Hence

$$\Delta j = \iiint \frac{g_1(\vec{k})}{\pi^3} \frac{q}{\hbar} \frac{\partial E}{\partial k_t} \cos \theta_t \, k^2 \sin \gamma \, d\gamma \, d\theta_t \, dk \tag{40}$$

In order to evaluate Δj, the expression given for $g_1(\vec{k})$ in equation (36) must be inserted in equation (40). This substitution gives

$$\Delta j = \frac{2}{\pi^2} \frac{q^2}{\hbar^3} \tau^2 \frac{\beta^2}{d^2} F \int dk \, d\gamma \, d\theta_t \, d\theta_t' \, k^2 \frac{1}{k_t} \frac{\partial f_0}{\partial k_t} \sin \gamma \cos \theta_t \frac{(\cos \theta_t - \cos \theta_t') \cos^2\left(\frac{\theta_t + \theta_t'}{2}\right)}{\sin^2\left(\frac{\theta_t - \theta_t'}{2}\right)} \tag{41}$$

Now $k_t = k \sin \gamma$. Furthermore,

$$\frac{\partial f_0}{\partial k_t} = \frac{df_0}{dk} \frac{k_t}{k} = \frac{df_0}{dk} \sin \gamma \tag{42}$$

Hence

$$\Delta j = \frac{2}{\pi^2} \frac{q^2}{\hbar^3} \tau^2 \frac{\beta^2}{d^2} F \int dk \, d\gamma \, d\theta_t \, d\theta_t' \, k \frac{df_0}{dk} \sin \gamma \cos \theta_t \frac{(\cos \theta_t - \cos \theta_t') \cos^2\left(\frac{\theta_t + \theta_t'}{2}\right)}{\sin^2\left(\frac{\theta_t - \theta_t'}{2}\right)} \tag{43}$$

Only near the top of the filled portion of the band is df_0/dk appreciably different from zero; hence it can be considered a negative Dirac δ function because all other terms in the integrand vary slowly with k. The integration over γ, from $\gamma = 0$ to $\gamma = \pi$, and the integration over k, from $k = 0$ to $k = \infty$, give

$$\Delta j = -\frac{4}{\pi^2}\frac{q^2}{\hbar^3}\tau^2\frac{\beta^2}{d^2}Fk_f\int d\theta_t\, d\theta_t'\cos\theta_t\,\frac{(\cos\theta_t - \cos\theta_t')\cos^2\left(\frac{\theta_t+\theta_t'}{2}\right)}{\sin^2\left(\frac{\theta_t-\theta_t'}{2}\right)} \tag{44}$$

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The particular value of k associated with the Fermi level is denoted by k_f. In appendix C the value of the integral is shown to be π^2. Therefore

$$\Delta j = -4\frac{q^2}{\hbar^3}\tau^2\frac{\beta^2}{d^2}Fk_f \tag{45}$$

and for the change in conductivity (absolute value is given)

$$|\Delta\sigma| = \frac{\Delta j}{F} = 4\frac{q^2}{\hbar^3}\tau^2\frac{\beta^2}{d^2}k_f \tag{46}$$

Now if there are N dislocations in the area d^2

$$\begin{aligned}|\Delta\sigma| &= 4\frac{q^2}{\hbar^3}\tau^2\beta^2 k_f\frac{N}{d^2}\\ &= 4\frac{q^2}{\hbar^3}\tau^2\beta^2 k_f\mathcal{N}\end{aligned} \tag{47}$$

where $\mathcal{N}$ is the number of dislocations per square centimeter.

Substituting the value of β given in equation (11) gives

$$|\Delta\sigma| = \frac{4}{9}\frac{a^2}{\pi^2}\left[\frac{1-\nu-2\nu^2}{1-\nu^2}\right]^2\frac{q^2}{\hbar^3}\tau^2 E_{B,0}^{\,2}k_f\mathcal{N} \tag{48}$$

The percentage change in conductivity is given by $|\Delta\sigma|/\sigma$. This is also the percentage change in resistivity, if the change is small. The value of σ is $nq^2\tau/m_0^*$ where m_0^* is the effective mass in the unperturbed lattice. Hence

$$\frac{|\Delta\sigma|}{\sigma} = \frac{|\Delta\rho|}{\rho} = \frac{4}{9}\frac{a^2}{\pi^2}\left(\frac{1-\nu-2\nu^2}{1-\nu^2}\right)^2\frac{\tau}{\hbar^3}E_{B,0}^{\,2}k_f m_0^*\frac{\mathcal{N}}{n} \tag{49}$$

Equation (50) gives the change in resistivity for current flow in the slip direction.

If the current flow is along the y-axis, that is, $\theta = \pi/2$, a slightly different computation applies. In equations (27), (28), and (32), k_x must be replaced by k_y. This substitution gives, instead of equation (34),

$$g_1(\vec{k}) = \tau^2 \frac{\partial f_0}{\partial k_t} \frac{qF}{\hbar} \int (\sin \theta_t - \sin \theta_t') P(\vec{k}',\vec{k}) \, dS'$$

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and an equivalent replacement in all subsequent equations. Equation (38) must be replaced by

$$v_y = \frac{1}{\hbar} \frac{\partial E}{\partial k_t} \sin \theta_t$$

Instead of equation (44), the following relation is then obtained:

$$\Delta j = -\frac{4}{\pi^2} \frac{q^2}{\hbar^3} \tau \frac{\beta^2}{d^2} Fk_f \int d\theta_t \, d\theta_t' \sin \theta_t \frac{(\sin \theta_t - \sin \theta_t') \cos^2\left(\frac{\theta_t+\theta_t'}{2}\right)}{\sin^2\left(\frac{\theta_t-\theta_t'}{2}\right)}$$

and in appendix C the value of the integral is shown to be $3\pi^2$, which gives

$$\frac{\Delta\sigma}{\sigma} = \frac{\Delta\rho}{\rho} = \frac{4}{3} \frac{a^2}{\pi^2}\left(\frac{1-\nu-2\nu^2}{1-\nu^2}\right)^2 \frac{\tau}{\hbar^3} E_{B,0}^{\,2} \, k_f \, m_0^* \frac{\mathcal{N}}{n}$$

In the z-direction, along the dislocation axis, the conductivity remains unchanged by the dislocation.

RESULTS

In a material in which dislocations occur with equal probability at all orientations, the increase in resistance is the average increase for the x, y, and z directions (reference 2). Hence for an isotropically cold-worked metal

$$\frac{\Delta\rho}{\rho} = \frac{16}{27} \frac{a^2}{\pi^2}\left(\frac{1-\nu-2\nu^2}{1-\nu^2}\right)^2 \frac{\tau}{\hbar^3} E_{B,0}^{\,2} \, k_f \, m_0^* \frac{\mathcal{N}}{n}$$

If the values given for copper in reference 4 are substituted,

$$\frac{\Delta\rho}{\rho} = 4.0\times10^{-14} \mathcal{N}$$

Setting this result equal to the 2-percent change usually observed in copper gives

$$\mathcal{N} = 5\times10^{11}/\mathrm{cm}^2$$

It is estimated (reference 6) that heavily cold-worked copper has 6×10^{11} dislocations per square centimeter. This estimate was based on stored-energy measurements. The agreement is excellent, indeed considerably better than the assumptions involved warrant.

The possibility that some of the stored energy may be in the form of screw dislocations has been neglected. In a simple cubic crystal, these dislocations are not accompanied by volume dilations and probably cause less scattering than edge-type dislocations. Furthermore, it should be taken into account that dislocations in a face-centered cubic metal, such as copper, occur in the form of half-dislocations.

Lewis Flight Propulsion Laboratory,
National Advisory Committee for Aeronautics,
Cleveland, Ohio.

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APPENDIX A

SYMBOLS

The following symbols are used in this report:

$A_0(\vec{r})$	solution of effective mass equation in undeformed crystal
$\lvert A_{k'} \rvert^2$	probability that transition from $\vec{k}$ to $\vec{k'}$ has occurred
a	slip distance
d	width of box (along z-axis) used in quantizing electron states
E	energy of electron in stationary state in perturbed periodic potential
E_B	width of filled portion of conduction band, function of position in vicinity of dislocation
$E_{B,0}$	width of filled portion of conduction band in unstrained metal
$E_{k'},E_k$	energies of final and initial state, respectively
F	electric field producing current flow
$f_0(\vec{k})$	probability that state $\vec{k}$ is occupied according to Fermi distribution
$f(\vec{k})$	probability that state $\vec{k}$ is occupied in the presence of electric field and dislocation
$g(\vec{k})$	deviation from Fermi distribution in normal undistorted lattice, in the presence of an electric field
$g(\vec{k}) - g_1(\vec{k})$	deviation from Fermi distribution in the presence of dislocation and electric field
h	Planck's constant
$\hbar$	$h/2\pi$
Δj	decrement in current due to dislocation
$\vec{k}$	wave vector of electron in initial state

$\vec{k}'$	wave vector of electron in final state
k_f	magnitude of $\vec{k}$ at top of filled portion of conduction band
$\vec{k}_t, \vec{k}_t'$	components of respective vectors that are perpendicular to dislocation axis
k_z, k_z'	components of respective vectors along dislocation axis
L	length of box (along z-axis) used in quantizing electron states
m_0^*	effective electronic mass in unstrained lattice
m^*	effective electronic mass, function of position in vicinity of dislocation
$M(\vec{k},\vec{k}')$	matrix element for transition from state $\vec{k}$ to state $\vec{k}'$ due to perturbation by dislocation
N	number of dislocations crossing area d^2
$\mathcal{N}$	number of dislocations per square centimeter
n	$n_0 + \Delta n$
n_0	number of ions per unit volume in unstrained metal
Δn	change in number of ions per unit volume due to strain, a function of position in vicinity of dislocation
$P(\vec{k},\vec{k}')$	probability per unit time that a transition from $\vec{k}$ to $\vec{k}'$ occurs
p	$E_{k'}-E_k/\hbar$
q	magnitude of electronic change
$\vec{r}$	position vector defining location with respect to an origin on dislocation axis
$\vec{r}_t$	component of $\vec{r}$ that is perpendicular to dislocation axis
dS	variable of integration in $\vec{k}_t$ space, dS is along a contour of constant energy
T	absolute temperature
t	time

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$\delta U(\vec{r})$	deviation of lower band edge from level at which it is when far away from dislocation
u	$1/2(\theta_t + \theta_t')$
v	$1/2(\theta_t - \theta_t')$
V_e	electrostatic potential whose scattering effect is equivalent to dislocation
V'	perturbing potential due to dislocation in wave equation
v_x, v_y	expectation value of electron velocity components
x,y,z	rectangular coordinates with z-axis along dislocation and x-axis in slip direction
α	$\theta - \theta_0$
β	$\frac{2}{3} \frac{a}{2\pi} \frac{(1-\nu-2\nu^2)}{(1-\nu^2)} E_{B,0}$
γ	angle that $\vec{k}$ vector makes with dislocation axis
ζ	Fermi level
θ	angle of elevation above slip plane, measured from dislocation axis
θ_0	angle $\vec{k}_t-\vec{k}_t'$ makes with slip plane
θ_t', θ_t	angles that $\vec{k}_t'$ and $\vec{k}_t$, respectively, make with the x-axis
κ	magnitude of $\vec{k}_t-\vec{k}_t'$
λ	rectangle of area d^2 perpendicular to dislocation axis
ν	Poisson's ratio
$d\xi$	variable of integration in $\vec{k}_t$ space; $d\xi$ is perpendicular to a contour of constant energy
ρ	resistivity of normal metal
$\Delta\rho$	change in resistivity caused by severe cold working
σ	conductivity of normal metal
$\Delta\sigma$	change in conductivity caused by severe cold working

τ	relaxation time for conduction process
$d\tau_{\vec{k}}$	volume element in $\vec{k}$ space
ψ_0	wave function for electron at bottom of conduction band

APPENDIX B

CHANGE OF ION DENSITY NEAR A DISLOCATION

The stress distribution surrounding an edge-type dislocation has been given in reference 7 as

$$
\begin{aligned}
p_{11} &= -D(\sin 3\theta + 3\sin\theta)/2r \\
p_{22} &= D(\sin 3\theta - \sin\theta)/2r \\
p_{12} &= D(\cos 3\theta + \cos\theta)/2r \\
p_{33} &= -D(4\nu\sin\theta)/2r \\
p_{13} &= p_{23} = 0
\end{aligned}
\tag{B1}
$$

where $D = Ga/2\pi(1-\nu)$, G being the shear modulus, and ν is Poisson's ratio. Now the strain tensor S_{ij} has diagonal terms given by

$$S_{ii} = \frac{1}{2G}\left(p_{ii} - \frac{p}{1+\nu}\,\epsilon\right) \tag{B2}$$

where p is the pressure, or the trace of the stress tensor, and ϵ is the unit tensor. The dilation is $\sum_i S_{ii}$ and is therefore given by

$$\sum_i S_{ii} = \frac{1}{2G}\left(p - 3\,\frac{p}{1+\nu}\right) \tag{B3}$$

Substituting from equation (B1) in equation (B3) gives

$$\sum_i S_{ii} = -\frac{a}{2\pi}\,\frac{(1-\nu-2\nu^2)}{(1-\nu^2)}\,\frac{\sin\theta}{r} \tag{B4}$$

The change in ionic density $\Delta n/n$ is the negative of equation (B4) and is given by

$$\frac{\Delta n}{n} = \frac{a}{2\pi}\,\frac{(1-\nu-2\nu^2)}{(1-\nu^2)}\,\frac{\sin\theta}{r}$$

APPENDIX C

EVALUATION OF INTEGRALS

The integral

$$\int_{-\pi}^{\pi}\int_{-\pi}^{\pi} d\theta_t \, d\theta_t' \cos\theta_t \frac{(\cos\theta_t - \cos\theta_t')\cos^2\left(\frac{\theta_t+\theta_t'}{2}\right)}{\sin^2\left(\frac{\theta_t-\theta_t'}{2}\right)} \tag{C1}$$

is to be evaluated. Let

$$\frac{1}{2}(\theta_t + \theta_t') = u \tag{C2}$$

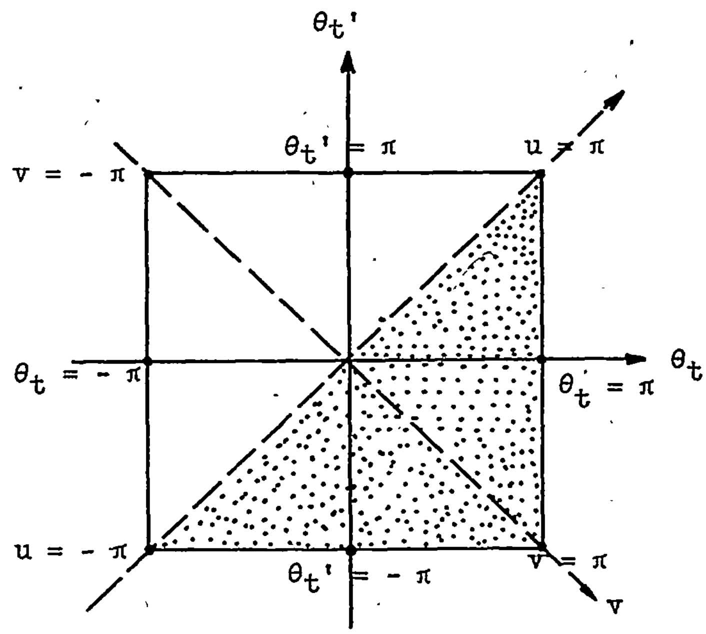
and

$$\frac{1}{2}(\theta_t - \theta_t') = v \tag{C3}$$

The integral given then becomes

$$\begin{aligned} &2\int_{v=0}^{\pi}\int_{u=v-\pi}^{u=\pi-v} du\, dv \left[\cos^2(u+v) - \cos(u+v)\cos(u-v)\right]\frac{\cos^2 u}{\sin^2 v} \\ &+2\int_{v=-\pi}^{v=0}\int_{u=-\pi-v}^{u=\pi+v} du\, dv \left[\cos^2(u+v) - \cos(u+v)\cos(u-v)\right]\frac{\cos^2 u}{\sin^2 v} \end{aligned} \tag{C4}$$

The factor 2 represents the Jacobian of the transformation. The range of integration is the square shown in the following figure:



The first integral ranges over the dashed triangle; the second integral over the remaining portion of the square. The terms in brackets can also be written

$$\left[2 \sin^2 u \sin^2 v - 2 \cos u \cos v \sin u \sin v\right] \tag{C5}$$

The first term of expression (C5) is even in v; the second is odd; $\cos^2 u/\sin^2 v$ is even in v. Therefore the first term of expression (C5) produces contributions of like sign and equal magnitude in the two integrals of equation (C4). The second term of expression (C5) produces contributions that cancel. Therefore expression (C4) reduces to

$$8 \int_{v=0}^{v=\pi} \int_{u=v-\pi}^{u=\pi-v} \sin^2 u \cos^2 u \, du \, dv \tag{C6}$$

The integral over u is a standard integral, listed in tables of integration. This integration leaves

$$\begin{aligned} \int_{v=0}^{\pi} \left(\frac{1}{2} \sin 4v + 2\pi - 2v\right) dv \\ = \frac{1}{8} \sin 4v + 2\pi v - v^2 \Big|_0^{\pi} \\ = 2\pi^2 - \pi^2 = \pi^2 \end{aligned} \tag{C7}$$

which is the value of (C1).

The integral

$$\int_{-\pi}^{\pi}\int_{-\pi}^{\pi} d\theta_t \, d\theta_t' \sin \theta_t(\sin \theta_t - \sin \theta_t')\frac{\cos^2\left(\frac{\theta_t+\theta_t'}{2}\right)}{\sin^2\left(\frac{\theta_t-\theta_t'}{2}\right)} \tag{C8}$$

is also to be evaluated. The transformation given by equations (C2) and (C3) must be used again and gives

$$2\int_{v=0}^{\pi}\int_{u=v-\pi}^{u=\pi-v} du\, dv\left[\sin^2 (u+v) - \sin (u+v) \sin (u-v)\right]\frac{\cos^2 u}{\sin^2 v} +$$

$$2\int_{v=-\pi}^{0}\int_{u=-\pi-v}^{u=\pi+v} du\, dv\left[\sin^2 (u+v) - \sin (u+v) \sin (u-v)\right]\frac{\cos^2 u}{\sin^2 v} \tag{C9}$$

The terms in the brackets can be written

$$\left(2 \cos^2 u \sin^2 v + 2 \sin u \cos v \cos u \sin v\right) \tag{C10}$$

As in expression (C1), only the term even in v contributes, leaving

$$8\int_{v=0}^{\pi}\int_{u=v-\pi}^{u=\pi-v} \cos^4 u \, du\, dv . \tag{C11}$$

After integration over u, the integral is

$$\int_{v=0}^{\pi}\left(6\pi - 6v - 4 \sin^2 v - \frac{1}{2} \sin 4v\right) dv$$

$$= 6\pi v - 3v^2 \Big|_0^{\pi} = 6\pi^2 - 3\pi^2 = 3\pi^2 \tag{C12}$$

which is the value of expression (C8).

REFERENCES

1. Bardeen, J., and Shockley, W.: Deformation Potentials and Mobilities in Non-Polar Crystals. Phys. Rev., vol. 80, no. 1, Oct. 1, 1950, pp. 72-80.

2. Mackenzie, J. K., and Sondheimer, E. H.: The Theory of the Change in the Conductivity of Metals Produced by Cold Work. Phys. Rev., vol. 77, no. 2, Jan. 15, 1950, pp. 264-270.

3. Koehler, J. S.: A Calculation of the Changes in the Conductivity of Metals Produced by Cold-Work. Phys. Rev., vol. 75, no. 1, Jan. 1, 1949, pp. 106-117.

4. Landauer, Rolf: Conductivity of Cold Worked Metals. Phys. Rev., vol. 82, no. 4, May 15, 1951, pp. 520-521.

5. Mott, N. F., and Jones, H.: The Theory of the Properties of Metals and Alloys, ch. VII, Oxford Press (London), 1936, pp. 240-314.

6. Koehler, J. S.: On Dislocation Theory and the Physical Changes Produced by Plastic Deformation. Am. Jour. Physics, vol. 10, no. 6, Dec. 1942, pp. 275-285.

7. Eshelby, J. D.: Dislocations as a Cause of Mechanical Damping in Metals. Proc. Roy. Soc., ser. A, vol. 197, June 22, 1949, pp. 396-416.

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